Development of Hourly Inventories Utilizing CEM-Based Data

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ABSTRACT

Recent improvements in emissions recording, reporting and modeling have allowed for analysis of some emission source types at an hourly level of temporal resolution. Continuous emissions monitoring (CEM) is the continuous measurement of pollutants emitted into the atmosphere in exhaust gases from combustion or industrial processes. The U.S. Environmental Protection Agency has established requirements for the continuous monitoring of SO2, volumetric flow, NOx, diluent gas, and opacity for units regulated under the Acid Rain Program. The CEM rule also contains requirements for equipment performance specifications, certification procedures, and recordkeeping and reporting. These recorded data can be used both directly and indirectly to allocate emissions to specific episodes of time during the emissions processing of inventories for air quality modeling analyses.

This paper describes the development of a set of calendar year 2002 hourly emission files and associated temporal allocation factors used in the VISTAS Phase II model performance evaluation specifically for modeling ozone and PM precursor power sector (EGU) emission inventories for national, annual episodes.

INTRODUCTION

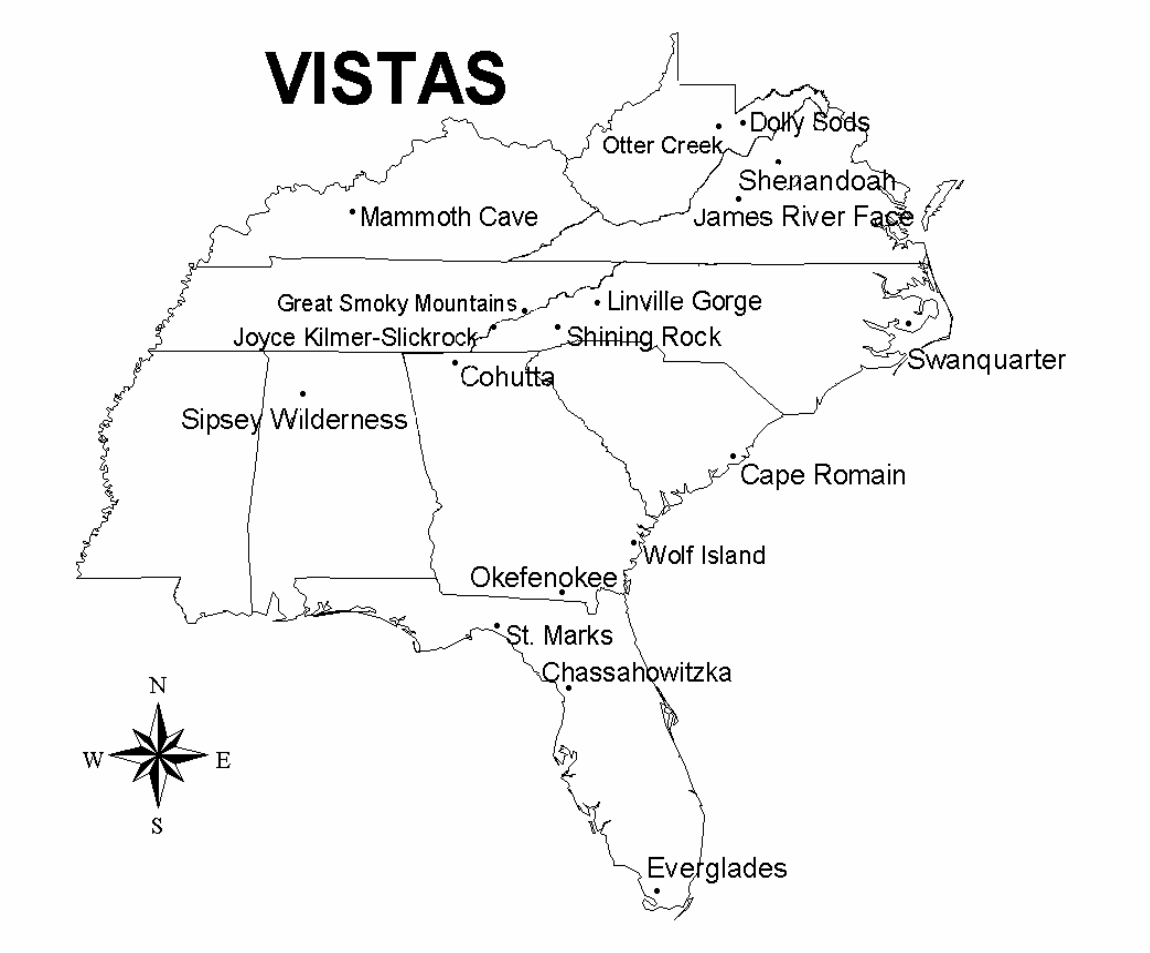
The Visibility Improvement State and Tribal Association of the Southeast (VISTAS) is a collaborative effort of state governments, tribal governments, and various federal agencies established to initiate and coordinate activities associated with the management of regional haze, visibility and other air quality issues in the Southeastern United States. It is one of five Regional Planning Organizations (RPOs) covering the U.S. that are developing a coordinated approach for addressing regional haze, fine particulate matter (PM) and ozone issues. VISTAS is comprised of the states of Alabama, Florida, Georgia, Kentucky, Mississippi, North Carolina, South Carolina, Tennessee, Virginia, and West Virginia as well as the Eastern Band of Cherokee Indians. The agencies participating in VISTAS are committed to a sound and thorough scientific analysis of regional haze problems, impacts from natural and man-made pollutants, and potential solutions. Stakeholders are encouraged to participate at the workgroup level in order that all aspects of the problem and possible strategies may be given consideration.

VISTAS has embarked on a multi-year effort to address the regional haze reduction requirements for the southeastern U.S. One of the components of VISTAS is the use of meteorological, emissions and regional PM/ozone models to project visibility at VISTAS Class I areas in future-years. The VISTAS modeling effort has been split into two Phases. Under Phase I, which was performed primarily in 2003, VISTAS tested and evaluated meteorological, emissions and PM/ozone models for three episodes to identify the optimal configuration for regional fine particulate, ozone and visibility modeling in the southeastern U.S. In Phase II, which was initiated in 2004, VISTAS is setting up and applying the selected models, guided by the Phase I research for the 2002 annual cycle and possibly additional periods.

The Phase II modeling entails detailed performance testing of the CMAQ modeling system followed by model applications to a variety of emissions control scenarios. These future year simulations are aimed

at enabling VISTAS to assess the effects of future year emission control strategies on visibility and other air quality issues. The modeling system will also allow VISTAS to track reasonable progress toward regional haze goals.

Figure 1. Class I areas within VISTAS domain.



VISTAS is also developing a comprehensive conceptual model of visibility impairment in the southeastern U.S. Brewer, Holman and Hornback[1] have reported a preliminary analysis to characterize the components of $PM_{2.5}$ and their contributions to visibility impairment in the VISTAS region. The analyses was based on monitoring data from the Interagency Monitoring of Protected Visual Environments (IMPROVE) network for the period 1998 to 2001 and from the Southeast Aerosol Research Characterization Study (SEARCH) network for the period 1999 to 2001. In both the IMPROVE and SEARCH networks, the 20% haziest days in the year occur most frequently in the summer and spring quarters and least frequently in the winter quarters. As can be seen in Figures 2 and 3, sulfate concentrations are the greatest contributor to light extinction at Class I areas in the VISTAS domain during the poorest visibility days. Figures 4 and 5 show similar contributions on the clearest days.

An annual 2002 CMAQ simulation using revised 2002 modeling inventories for VISTAS and non-VISTAS States, Canada and Mexico was performed in late 2004. The primary objective of this run was model performance demonstration using updated emissions inventories and model configuration refinements.

Figure 2. Components of average light extinction (Mm^{-1}) at southeastern U.S. IMPROVE monitors for the 20% poorest visibility days from 1998-2001.

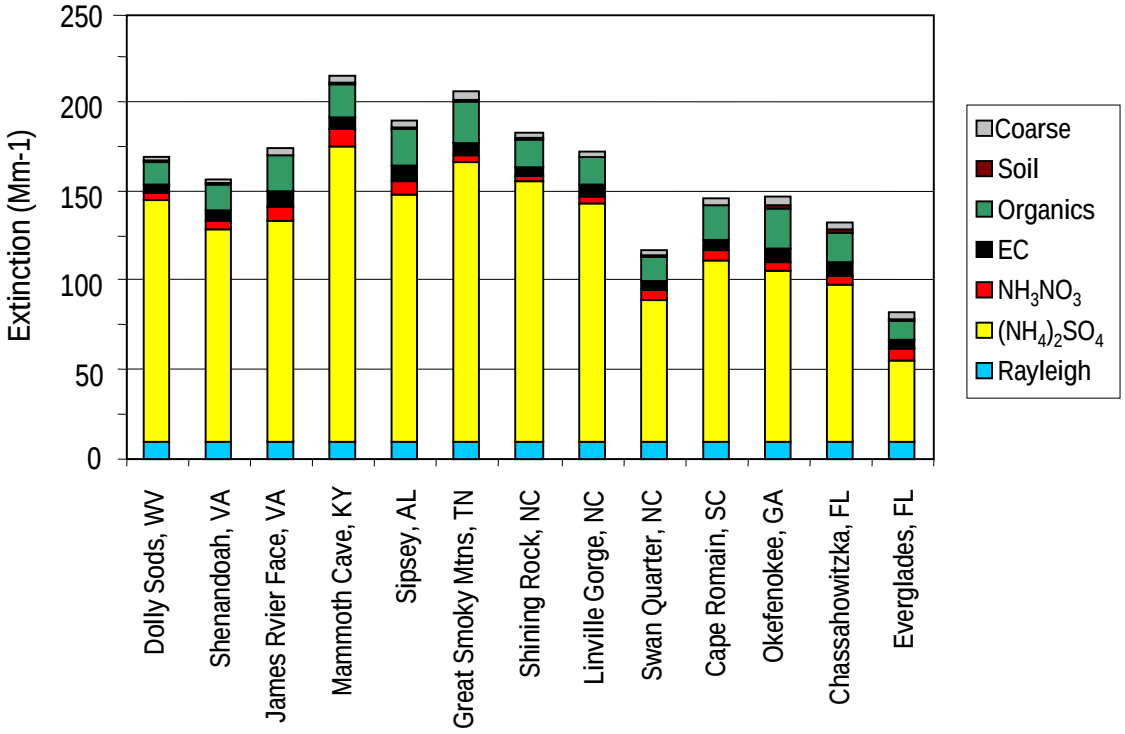


Figure 3. Components of average light extinction (Mm^{-1}) at southeastern U.S. SEARCH monitors for the 20% poorest visibility days from 1998-2001.

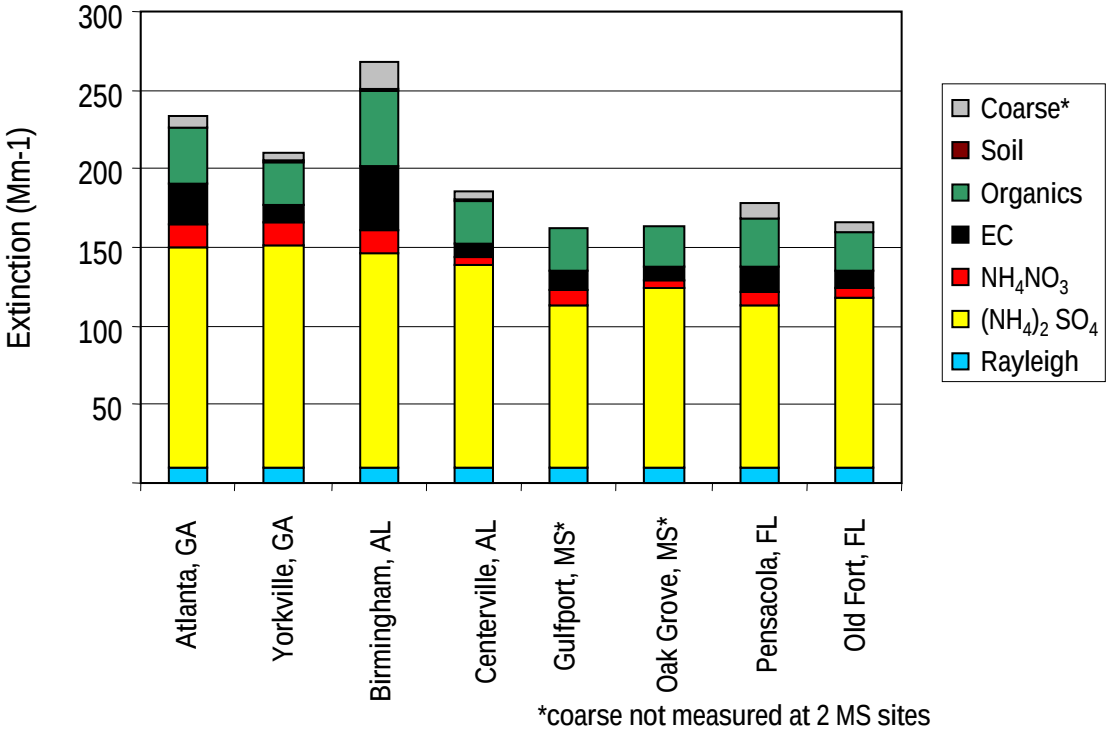


Figure 4. Components of average light extinction (Mm^{-1}) at southeastern U.S. IMPROVE monitors for the 20% best visibility days from 1998-2001.

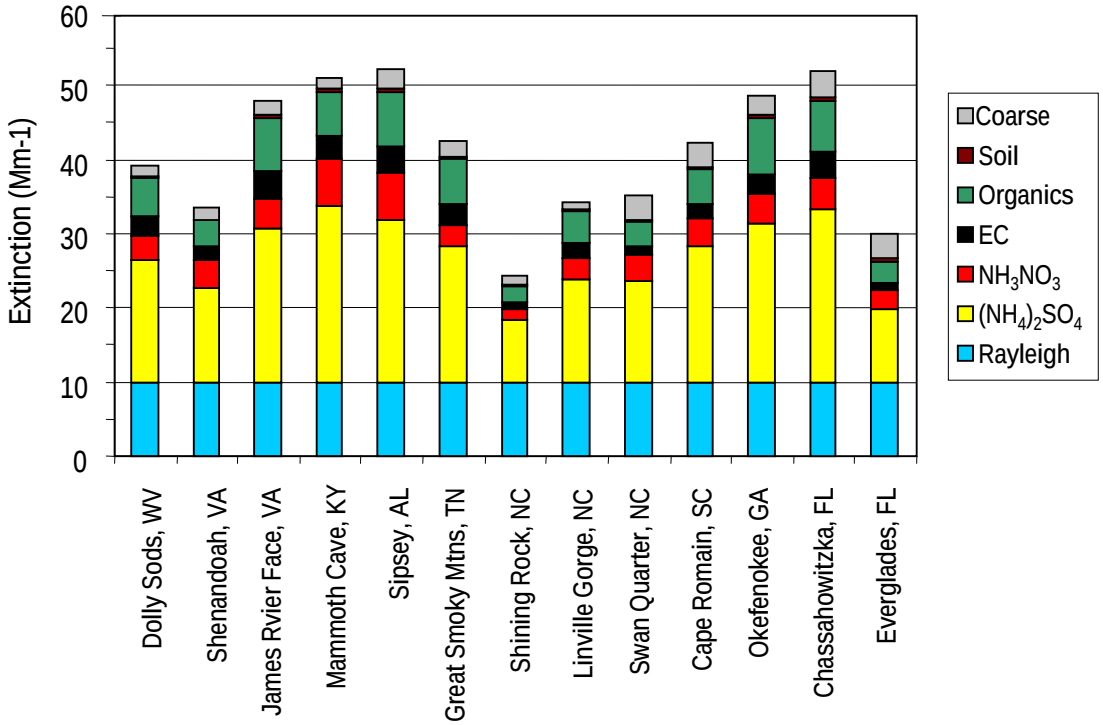
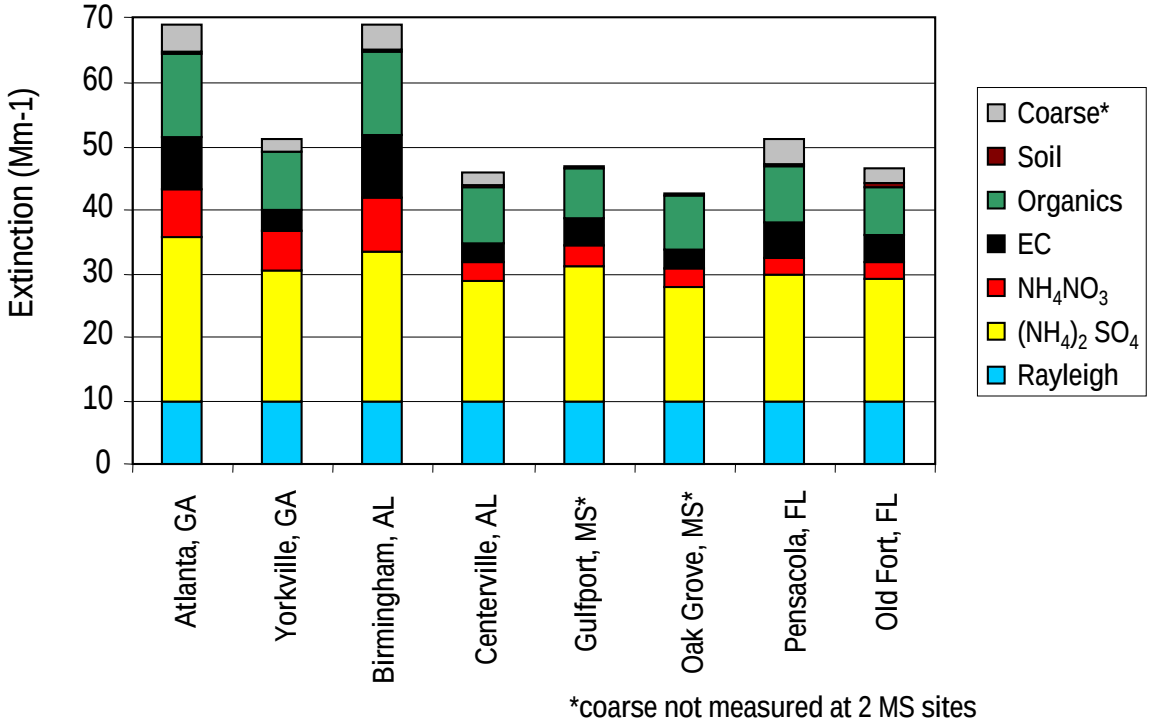


Figure 5. Components of average light extinction (Mm^{-1}) at southeastern U.S. SEARCH monitors for the 20% best visibility days from 1998-2001.



The contribution of individual source types to the degradation of visibility in the Class I areas is estimated most reliably by modeling each source with as fine a temporal resolution as possible. Recent improvements in emissions recording, reporting and modeling have allowed for analysis at an hourly level of temporal resolution. Continuous emissions monitoring (CEM) is the continuous measurement of pollutants emitted into the atmosphere in exhaust gases from combustion or industrial processes. The U.S. Environmental Protection Agency has established requirements for the continuous monitoring of SO2, volumetric flow, NOx, diluent gas, and opacity for units regulated under the Acid Rain Program. The CEM rule also contains requirements for equipment performance specifications, certification procedures, and recordkeeping and reporting. These recorded data can be used both directly and indirectly to allocate emissions to specific episodes of time during the emissions processing of inventories for air quality modeling analyses.

In the following sections, the development of a set of calendar year 2002 hourly emission files and associated temporal allocation factors used in the VISTAS Phase II modeling are discussed. The hourly data sets figure prominently in CMAQ modeling assessments of the role of power sector (EGU) emissions on 8-hr ozone and fine particulate impacts throughout the U.S.

BASE YEAR 2002 EGU EMISSION INVENTORY DEVELOPMENT

Through other contracts, VISTAS had previously funded the development of base year 2002 emission inventories for all anthropogenic sources. In late 2004, second generation annual inventories of VOC, NOX, CO, SO2, PM-10, PM-2.5, and NH3 were completed and delivered to VISTAS for EGU, non-EGU point, stationary area, onroad and nonroad mobile, and fire source categories.

The data sets used to develop these initial base year inventories originated from the VISTAS State Consolidated Emission Reporting Rule (CERR) requirements supplemented with additional unit or pollutant specific adjustment based on State, local, or stakeholder comments. The data were prepared in a form (National Emission Inventory Input Format 3.0) and a time period (annual) as submitted to fulfill this reporting obligation. Each step of the process was quality assured by VISTAS stakeholder workgroups and State emission inventory developers. These emissions data were developed with the intent to support the regional modeling exercises planned by VISTAS and its States.

Table 1. Ten State VISTAS domain annual 2002 emissions (tons) – selected pollutants.

	2002 Annual Emissions (Tons)			**Percent of 2002 Total**		
Source Category	**NOx**	**SO2**	**PM-10**	**NOx**	**SO2**	**PM-10**
Fuel Comb. Elec. Util.	1,514,950	3,720,703	111,810	29%	78%	3%
Fuel Comb. Industrial	484,885	449,373	112,110	9%	9%	3%
Fuel Comb. Other	106,405	109,595	100,218	2%	2%	3%
Chemical & Allied Product Mfg	20,366	77,450	10,733	<1%	2%	<1%
Metals Processing	11,904	49,367	28,992	<1%	1%	1%
Petroleum & Related Industries	7,112	53,381	2,425	<1%	1%	<1%
Other Industrial Processes	116,839	97,586	84,945	2%	2%	2%
Solvent Utilization	5,675	92	4,315	<1%	<1%	<1%
Storage & Transport	1,071	232	8,798	<1%	<1%	<1%
Waste Disposal & Recycling	30,042	6,186	120,019	1%	<1%	3%
Highway Vehicles	2,152,993	87,167	50,393	41%	2%	1%
Off-highway	799,063	89,168	69,514	15%	2%	2%
Miscellaneous	44,089	11,344	3,089,978	1%	<1%	81%
Total	**5,295,394**	**4,751,644**	**3,794,249**	**100%**	**100%**	**100%**

From Table 1, almost eighty percent of SO2 and thirty percent of NOx emissions in the VISTAS ten state domain are attributed to the electric generating power sector. Since the largest of these sources are required to operate CEMs, data are available to develop a relatively accurate accounting of these emissions on an hourly basis for the period of interest.

CEM DATA

Through the EPA's Clean Air Market's Data and Maps website[2], quarterly unit-level hourly emissions data by State and calendar year 2002 were obtained for purposes of developing temporal allocation factors applicable to EGU sources within the VISTAS domain. Key elements in these data sets include the State where the unit is located, facility name, facility identification (ORISPL) code (assigned by the Department of Energy at the Energy Information Administration), unit identification code, date of record, hour of record, SO2, CO2, and NOx mass (in lbs per hour), heat input (million British thermal units [MMBtu]), and NOx emission rate (lbs/MMBtu).

SO2 and NOx mass and heat input values were summed for each unit to an annual level to allow for the calculation of an hour of date-to-annual ratio estimation. Equation 1 provides this calculation for heat input.

Equation (1) $$hi_{ratio,hr,date} = hi_{hr,date} \Big/ \sum_{Dec31}^{Jan1} hi$$

where hi = heat input (MMBtu)

Since it was assumed that all sources in the VISTAS EGU inventory would not be matched to individual CEM-based units, the same calculations were performed for each facility and State so that a hierarchical application of ratios (unit first, facility second, State third) could be assigned as necessary.

Three parameter values (SO2 mass, NOx mass, heat input) were calculated at each aggregation as NOx and SO2 emissions vary due to fuel blend, sulfur content, or seasonal control and are not necessarily representative of the other variables' seasonal, daily, or even hourly variation. As seen in Figure 6, when viewed on a VISTAS-domain total, the monthly variation in relative distribution of SO2, NOx, and heat input differs enough to justify calculating each parameter value set of temporal profiles with CEM data.

When viewed on a State by State basis, the differences in monthly variation are even more pronounced as individual facilities within each State may be affected during any calendar year by extreme temperature variation, shutdowns, or regular maintenance or installation of equipment. Figure 7 represents CEM data from the State of Mississippi during calendar year 2002 and reveals that SO2 emissions increase throughout the year, NOx emissions stay relatively high during the summer months, and heat input peaks during the month of July. Although Figures 6 and 7 are roughly comparable in shape and monthly distribution, the relative distribution of these values are quite different. In Mississippi's case, close to thirteen percent of the State's CEM-based heat input occurs in July. This compares to the VISTAS average of just over ten percent of CEM-based heat input in July.

Figure 6. Monthly variation in 2002 of CEM reported heat input, NOx mass, and SO2 mass for VISTAS domain.

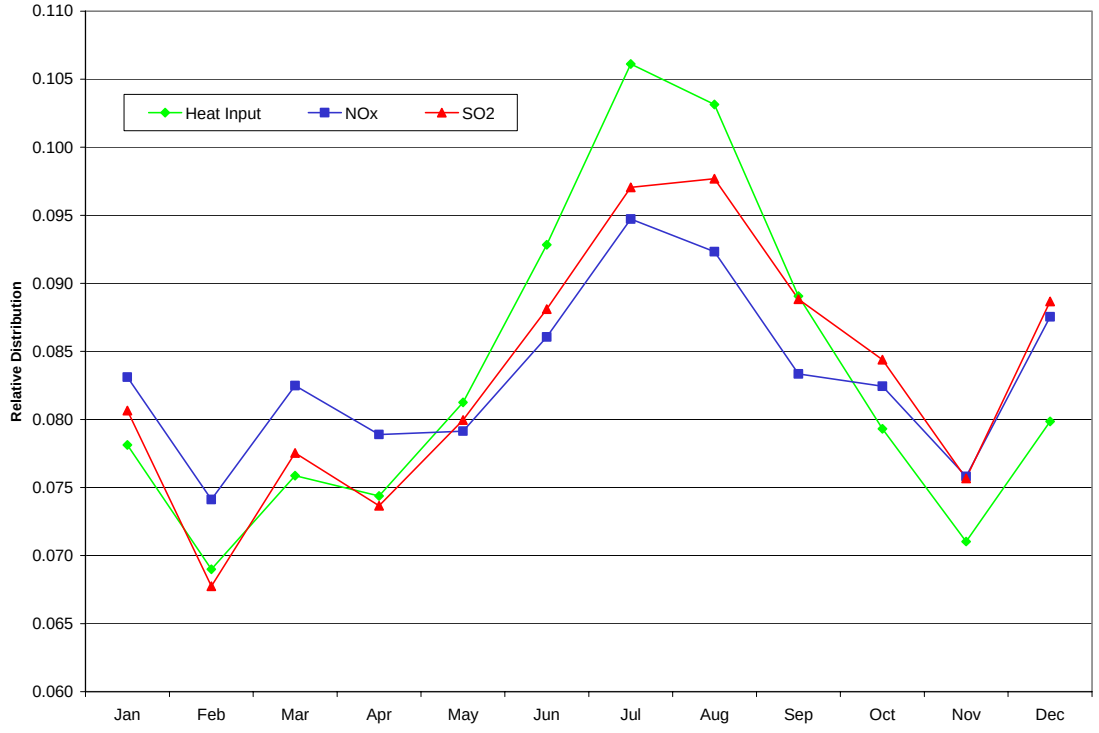
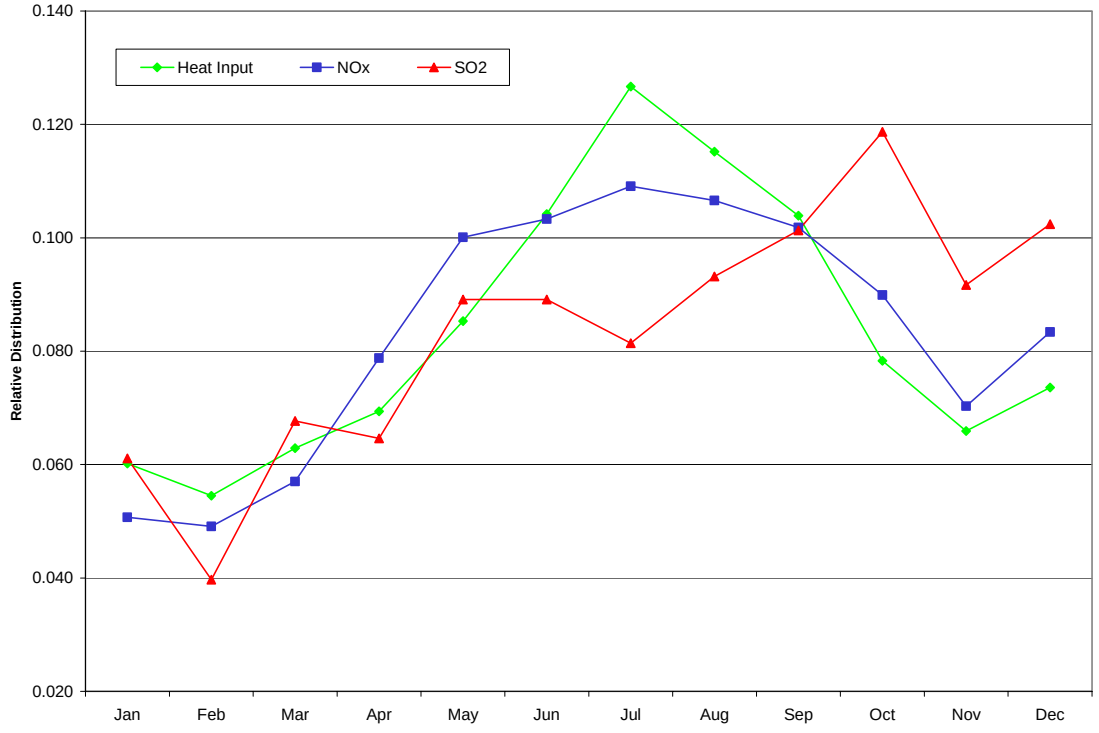


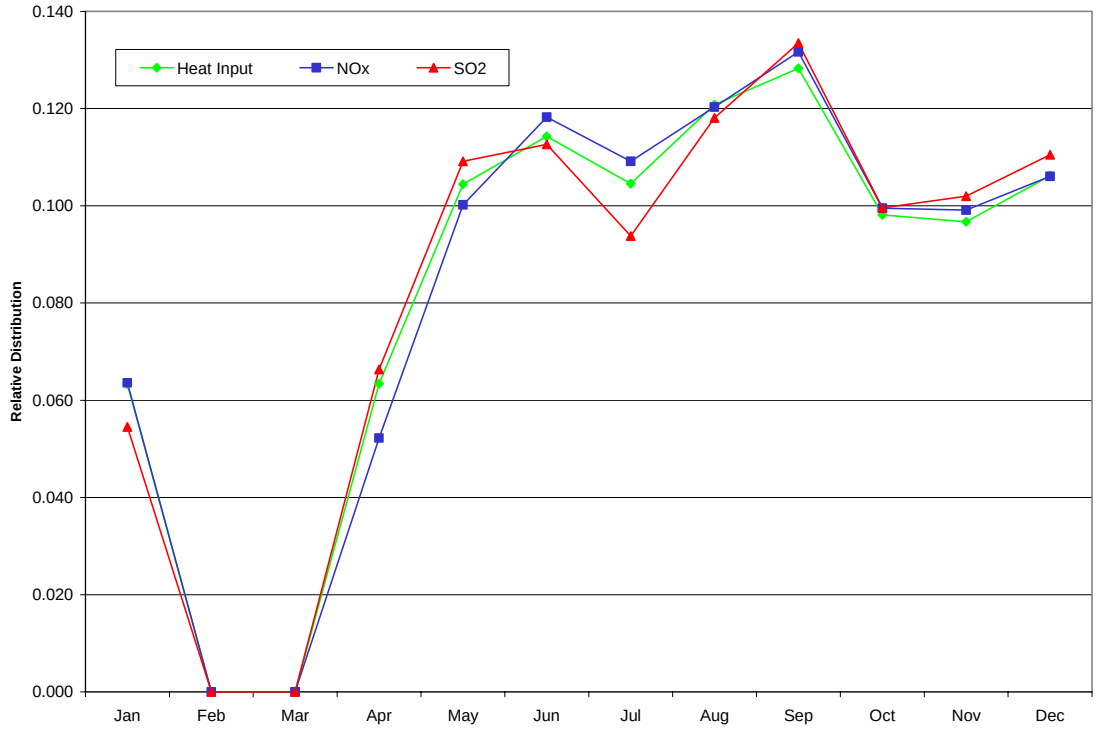
Figure 7. Monthly variation in 2002 of CEM reported heat input, NOx mass, and SO2 mass for Mississippi.



Finally, when these data are reviewed at a unit level, the differences become incrementally more distinct due to the unique nature of individual facilities, their operating schedules, pollution regulation, fuel characteristics, and applied technologies. For example, a facility that is complying with summertime NOx regulation may have selective catalytic reduction (SCR) installed on its boiler(s) which in practice may only be run during ozone season months. During this period of time, heat input and SO2 emissions may remain consistent with State or regional monthly profiles, but the NOx emissions may drop significantly relative to the rest of the year.

Figure 8 represents an extreme unit-specific case for monthly differences from State or regional temporal allocation. The unit presented is a Mississippi baseload coal-fired boiler which in 2002 emitted over 4,000 tons of NOx and over 11,000 tons of SO2. This unit would typically run at consistent levels during the entire period, but due to a planned maintenance outage was not in operation in late January through the middle of April. Given the unique operation of this boiler during 2002, the use of a regional or even State-level monthly temporal distribution would introduce significant inaccuracy to air quality modeling in the immediate or downwind area associated with this facility. While this may not be significant at great distance downwind of the source or for annual concentration estimates, more locally, and especially over shorter time scales (daily or weekly), such simplifications would have a noticeable effect on air quality model predictions.

Figure 8. Monthly variation in 2002 of CEM reported heat input, NOx mass, and SO2 mass for specific baseload coal-fired unit in Mississippi with planned outage in late January through mid April.

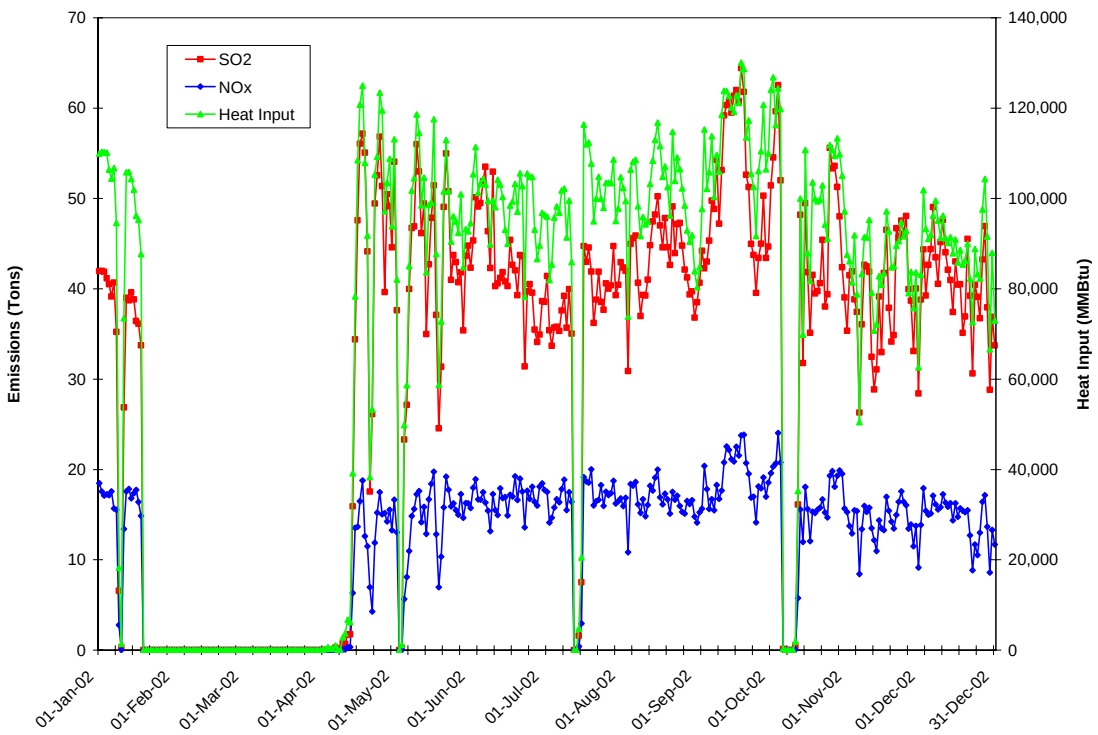


Thus, while improving the representativeness of unit-specific monthly temporal profiles is desirable, providing day and hour-specific values are clearly better. For this reason, during the model performance evaluation process in the VISTAS Phase II modeling, hour-specific temporal ratios were developed for every CEM reporting unit in the VISTAS domain. These ratios allowed for the hour-by-hour accounting

of emissions released at each unit at each facility within the VISTAS domain that reported output under the CEM guidelines.

Figure 9 represents the actual daily distribution of SO2 and NOx emissions and heat input from the Mississippi baseload unit from the above example. As can been seen in this figure, not only is the planned January through April outage represented correctly, there are significant peaks and valleys throughout the calendar year which could not be accurately represented with the application of average monthly, day-of-week, or hourly distribution factors. In reality, only the actual operating characteristics of this unit could capture the differences from hour to hour which are potentially quite important in terms of correctly modeling the impact of the source on downwind oxidant and fine particulate concentrations.

Figure 9. Actual daily unit-specific 2002 SO2 (tons), NOx, (tons), and heat input (MMBtu) distribution from CEM data.



INVENTORY MATCHING

Once the unit-specific SO2, NOx, and heat input ratios were developed for each hour of calendar year 2002, the step of matching CEM units to the VISTAS 2002 modeling inventory started. Because naming convention and facility or unit numbering can be unique at the Federal, State, local, or facility level, the step of matching existing units from an emissions inventory to the CEM data base proved to be more complicated than anticipated.

Recall from Table 1 that the VISTAS EGU emission inventory accounted for approximately 3.7 million tons of SO2 and 1.5 million tons of NOx in calendar year 2002. There were 861 units reporting to the CEM database in 2002 for the ten VISTAS States. The primary objective of the inventory matching

steps was to account for as many units and tons as possible allowing for the unit-specific application of hourly temporal distribution profiles.

Under the direction of VISTAS, staff at MACTEC Engineering and Consulting, Inc. prepared comparisons of the VISTAS 2002 emission inventory of EGU sources to that of CEM-based emissions, heat input, and operating characteristics. For each unit identified as an EGU source in the VISTAS inventory, an attempt was made to match it to a CEM unit and associated data.

Automated facility (ORIS) and unit identification was made for a majority of units who maintained the same numbering and nomenclature between the two data sets. This first computerized step captured the majority of emissions by matching some of the largest units in the VISTAS domain. The remaining steps were followed in order to match the outstanding facilities and emissions as reported by VISTAS States in the 2002 emission inventory.

MACTEC developed county-level reports of the remaining unmatched facilities and units from the VISTAS inventory and made comparisons of annual emissions of SO2 and NOx to the CEM-based SO2 and NOx for sources also identified within the same county. This step of the matching process allowed an incremental amount of emissions and units to be accounted for and assigned unit-specific profiles for model performance evaluation.

Finally, remaining VISTAS inventory and CEM sources were manually compared to each other in an effort to determine if reporting errors in State or county codes or facility or unit identification codes accounted for this reminder of unmatched sources. These manual matches were confirmed or revised with VISTAS State and stakeholder participation and input. With this step, a few sources were identified to have facility identification changes or misreported county codes preventing automated matching from occurring and corrected for the final application of factors.

Once all methods of comparison were exhausted, the remaining unmatched VISTAS emission inventory of EGU sources was excluded from the unit-specific profile assignment steps and were allocated more generalized facility or State temporal profiles as described in the following section.

This inventory comparison process allowed for the match of over 650 of the 861 CEM identified units (76%) to the VISTAS EGU emission inventory for 2002. More importantly, however, was the match of 99.95 percent of the SO2 emissions and over 99.4 percent of the NOx emissions from these sources in the VISTAS domain.

APPLICATION OF FACTORS

VISTAS chose to prepare its air quality modeling inventories with Version 2.0 of the Sparse Matrix Operating Kernel Emissions (SMOKE) model. For this reason, all emissions were required to be converted to SMOKE's particular data formats. In particular, because hour specific temporal profiles for each day of a year are not accepted directly by the model, it was necessary to develop a set of hourly emissions inputs to circumvent this limitation. These were generated in the EMS PTHOUR format as described in SMOKE input file documentation[3].

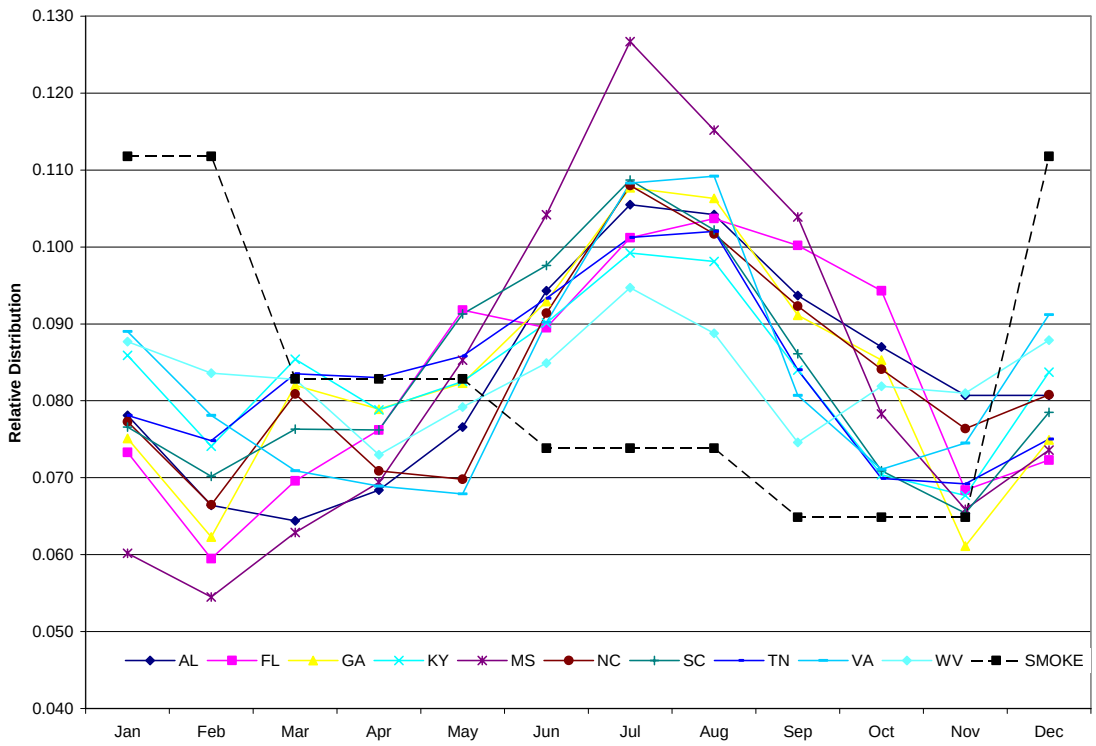
The CEM format for individual hour-specific data files as available in SMOKE was not utilized for VISTAS emissions processing as the emissions allowable by hour would have been limited to NOx, SO2, and CO2. If this file format and optional run configuration were exercised, the NOx, SO2, and

CO2 emissions processed by the model would have been accurate, but the remaining pollutants coupled with each CEM unit would have received the monthly, daily, and diurnal temporal profiles associated with the source category codes from the unit. This could lead to potentially displaced emissions if a unit were operating at different times than the default profiles indicated.

In VISTAS Phase II modeling, for those EGU sources where CEM data were utilized, NOx, SO2, and heat input-based hour-specific profiles were developed and applied to annual NOx, SO2, and all other emissions, respectively. Heat input was chosen as a surrogate for non-CEM reported pollutants as the majority of remaining compounds are not as significantly impacted by controls or fuel content, yet the distribution of these emissions would occur during the same times CEM reported pollutants were emitted.

The application of hourly ratios to annual emissions ensured that the annual values provided by States under the CERR were maintained, but distributed using actual hourly to annual profiles. Additionally, for stakeholder sources providing hour-specific data approved by the State in which they operated, data were substituted for State provided emissions and CEM-based distributions.

Figure 10. Relative distribution of monthly VISTAS State CEM-based heat input.



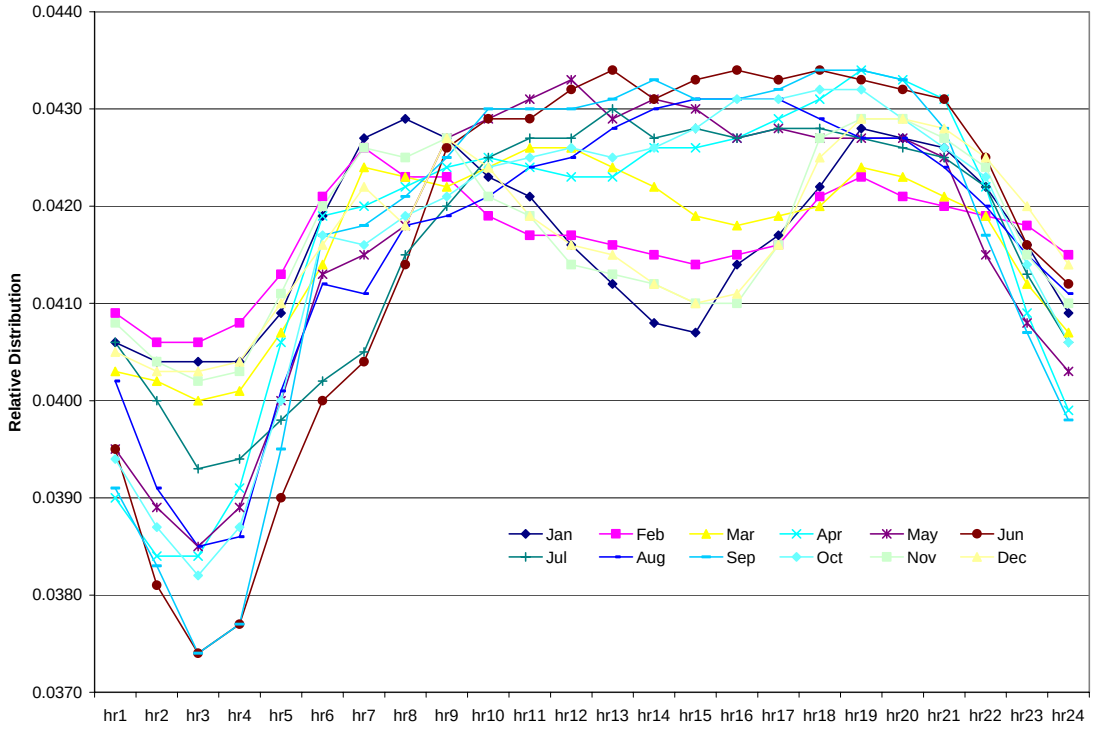
To temporally allocate the remaining EGU point sources, the NOx, SO2, and heat input data were collected from the 2002 CEM datasets, and used to develop State-level temporal distributions. These month-specific hour and day of week temporal profiles were used in conjunction with the emissions inventory to calculate hourly EGU emissions by unit.

Although not as accurate a distribution as the unit-specific factors, the State-based temporal distribution provided improved results to the default profiles provided with the emissions model. Figure 10 represents the monthly distribution comparisons of VISTAS State heat input to the default monthly distribution from Version 2 of SMOKE for source category code (SCC) 10100201, representing

External Combustion Boilers; Electric Generation; Bituminous/Subbituminous Coal; Pulverized Coal: Wet Bottom (Bituminous Coal), a relatively common boiler type and fuel configuration in the VISTAS domain.

Much like the distinction in month to month variation of the profiles, day of week and diurnal patterns based on CEM data vary from unit to unit. Again, if one were to assign the same day of week or diurnal profile to every unit in the inventory, emissions from these sources would inappropriately be distributed during the episode of interest. In addition to the unique distribution provided by the unit-specific factors based on CEM data, aggregate State level daily and diurnal temporal distribution factors were developed and applied during this process. Figure 11 shows the variance in diurnal distribution from Tennessee's average CEM-based NOx emissions data for each of the twelve months of calendar year 2002 as would have been applied to units unmatched to CEM sources.

Figure 11. Relative distribution of diurnal 2002 CEM-based NOx emissions for Tennessee.



RESULTS

Application of the CEM-based temporal profiles to annual emission totals at the unit or State level for facilities in the VISTAS domain exhibit the uniqueness of individual sources and their operating characteristics. This hourly distribution of emissions greatly enhanced the inputs provided to the air quality model and improved model performance in more than one season and sub episode.

As seen in Figure 12, CEM-allocated SO2 emissions for the domain have distinct high and low points compared to the application of default temporal profiles to these same sources. During the months of February through May and late October through November, application of the default temporal profiles

would have over estimated SO2 emissions in the domain while significantly underestimating SO2 in early January and December and in the months of June through September.

Similar results are seen in Figures 13 and 14, representing NOx and PM-10 emissions, respectively. The seasonal differences exist during the same periods as in the SO2 example, consistent with the activity of these sources during the episode.

Figure 12. VISTAS domain EGU SO2 emissions with and without CEM-based allocation factors.

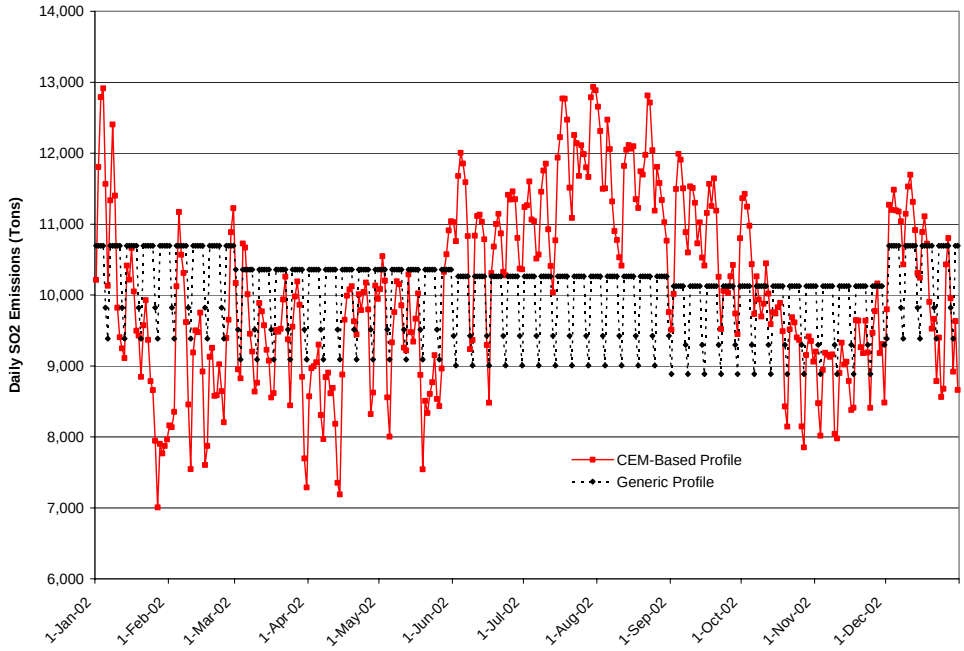


Figure 13. VISTAS domain EGU NOx emissions with and without CEM-based allocation factors.

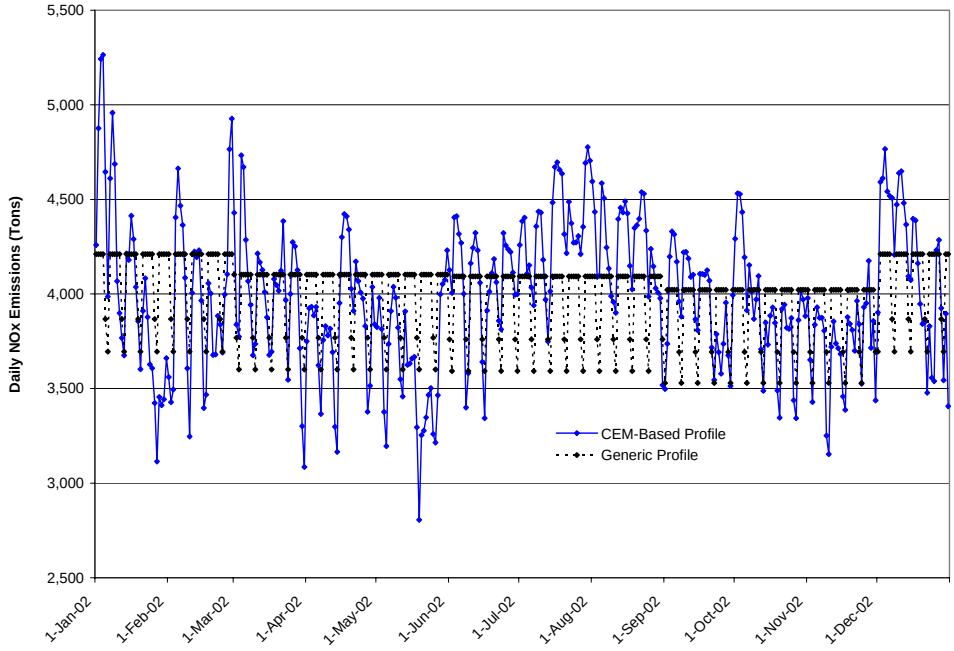
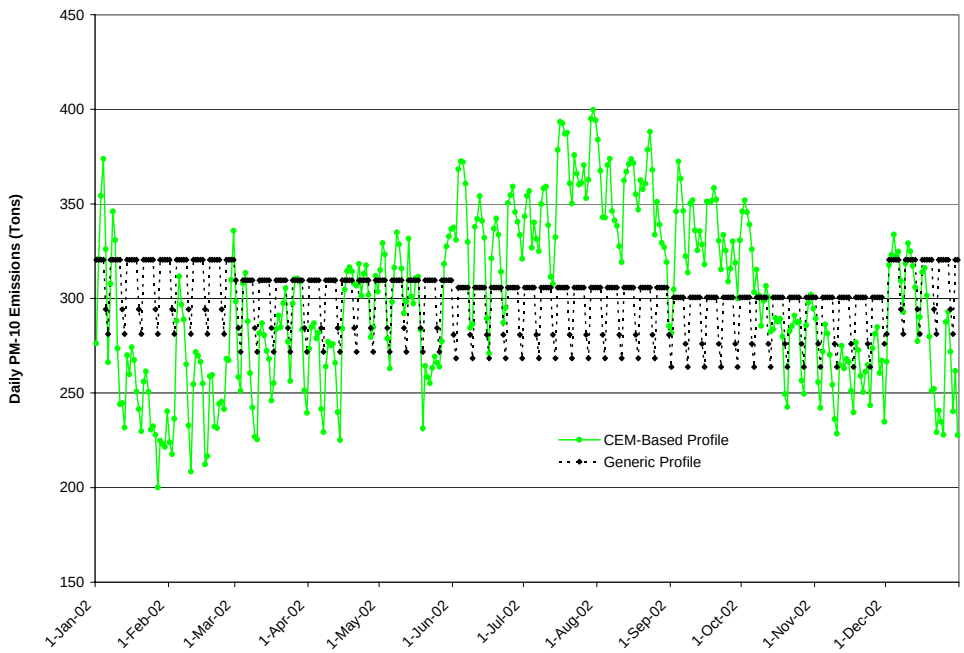


Figure 14. VISTAS domain EGU PM-10 emissions with and without CEM-based allocation factors.



CONCLUSIONS

Rigorous evaluation of regional ozone/fine particulate air quality models requires not only focused testing of the host air quality model but also an examination of the supporting emissions and meteorological pre-processor programs and their attendant input data sets. If one of the measured or modeled parameters is imprecise or incorrectly estimated, the air quality model's performance might be judged inadequate for the wrong reason. The model itself may be technically sound, but if the inputs are erroneous, the reliability of the model predictions will suffer. Even more vexing is the existence of compensatory errors where two sets of model inputs are incorrectly prescribed but their errors cancel, yielding performance that appears to be good but for the wrong reasons. Models containing such compensating errors have been shown to produce quite misleading future year control strategy results when the balance between the two erroneous inputs become altered in the future simulation. Largely for this reason, emission inventories for regulatory air quality modeling should be compiled at the most highly resolved temporal and spatial scales as possible.

Our research with the VISTAS inventories and other studies has demonstrated that the use of actual hourly emissions is indeed valuable. However, today's mechanisms and procedures for collecting and reporting these emissions and associated data are limited to a few source types.

The utilization of CEM-based temporal profiles allows for this best modeling practice with respect to EGU emissions. The hour by hour accounting of operation and emission from some of the largest SO2 and NOx source emitters clearly enhances the reliability of chemical transport model predictions and the provides technical support for policy makers increased confidence in decisions on future strategies based on air quality simulations.

The application of SO2, NOx, and heat input-based hourly distribution factors allows for the most accurately available accounting for CEM-based EGU emissions during episodes of interest. In VISTAS

Phase II modeling and model performance evaluation for calendar year 2002, these hourly estimates of sulfate and nitrate forming pollution sources have been demonstrated to improved model performance, thereby affording increased confidence in the control strategy evaluation results.

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KEYWORDS

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EGU
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Regional Haze
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VISTAS